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Theoretical Study of the Dissociation of Small Neon Clusters

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Theoretical study of the dissociation of small neon clusters

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The Molecular Dynamics with Quantum Transitions method (MDQT) is applied to investigate the dynamics of the dissociation of smal ionized neon clusters (up to 7 atoms). The motion of the neon atoms is treated classically, while transitions between the different potential energy surfaces (PES) of the ionic clusters are treated quantum quantum mechanically. These PES are generated using the semiempirical diatomics-in-molecule method (DIM) applied to a minimal basis set consisting of the 2p orbitals of each neon atom, in addition the induced dipole-induced dipole interaction is taken into account.

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